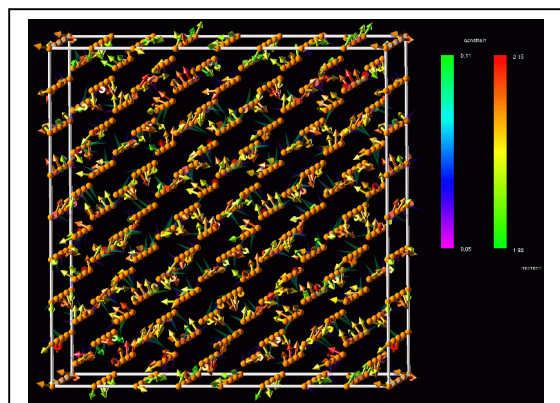# VI.A First Principles Studies of Finite Temperature Magnetism

Introduction: Understanding and predicting the properties of magnetic materials is essential for optimizing the design of power generators, motors, and essentially all devices containing permanent magnets. New magnetic materials have made lightweight tiny motors (for cameras, car windows, and electric pencil sharpeners) a part of everyday life. Yet magnet performance is far from reaching known theoretical limits. There has been no method for using the quantum mechanical (QM) interactions governing magnetism at the atomic level to predict practical properties. Recently, new approaches have been developed that permit full QM treatment of thousands of magnetic atoms at finite temperature. The illustration at left shows atomic magnetic moments at high temperature. At low temperatures, the moments are aligned. The magnitudes of the moments and the fields can now be precisely evaluated for complicated situations.

**Magnetic moments and local magnetic fields
for a model of Iron at high temperature**

Calculational Notes: Calculations were performed using the Locally Self-consistent Multiple Scattering (LSMS) method. The calculation shown is for a 512 atom per unit cell array of moments and was performed on the 512 node SGI-Cray T3E at NERSC. The research won the 1998 Gordon Bell Prize for "Best Performance of a Supercomputer Application."
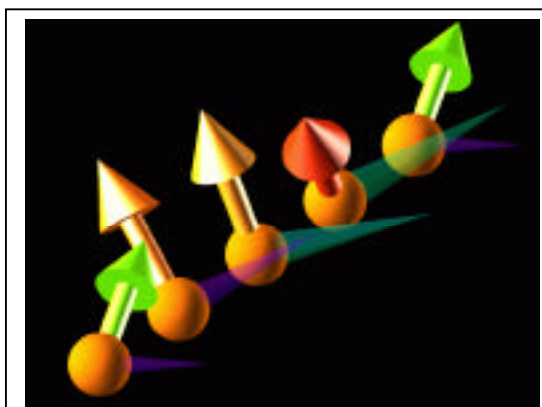
**Detail taken from upper illustration showing
relationship between magnetic moments and
magnetic fields**

Results: The upper illustration is a snapshot of the results of calculations of the magnetic moments (arrows) and forcing fields (translucent spikes) for a model of iron above its magnetic ordering temperature. In the calculation, the magnetic moments and resulting forcing fields are obtained entirely from first principles calculations (i.e., using no empirical parameters). The lower illustration is a blowup of a few of the sites in the upper illustration, allowing a better view of the detailed relationship between moments and forcing fields.

Significance: The ability to accurately treat a large number of magnetic atoms will allow detailed evaluation of the interactions among moments near defects. The defects can pin the magnetic moments in a good permanent magnet and keep them from changing direction. Understanding of these interactions will provide needed information for micromagnetic modeling tools so that scientists will finally be able to understand the detailed relationship between a material's microstructure and its bulk magnetic properties. SSI levels of computing power are essential to consider extended defects, which are known to enhance permanent magnet performance and for integrating with micromagnetics.